SVDs in 3D and Beyond

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Norms

$$
\begin{aligned}
\|\mathbf{y}\|_2 &= \sqrt{\{|y_1|^2 + |y_2|^2 + \ldots + |y_n|^2\}} \\
\|A\|_2 &= \max_{\|\mathbf{y}\|=1} \|A\mathbf{y}\|_2 \quad \text{2-norm} \\
\|A\|_{\mathsf{F}}^2 &= \sum_{i=1}^{m} \sum_{j=1}^{n} |a_{ij}|^2 \quad \text{Frobenius norm} \\
\|A\| &= \text{either } \|A\|_2 \text{ or } \|A\|_{\mathsf{F}}
\end{aligned}
$$

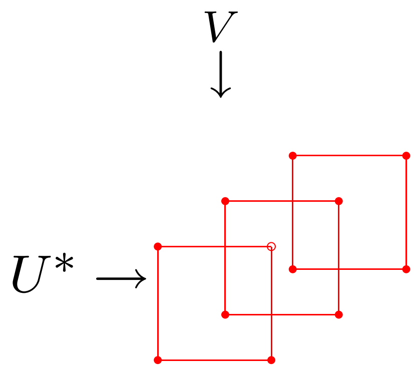
Classical Tensor Notation

- too many indices
- too many summations
- multiplications can be tedious
- can be clumsy
- far away from matrix notation

A 3D Array

- a 3D array can be sliced
- each slice is a matrix (2D array)
- each matrix = a set of data
- each matrix = a cross-section of data
- each matrix = an image

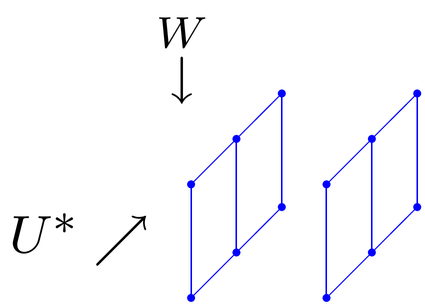
Slicing an $m \times n \times p$ Array Θ



$m = n = 2 \ , \ p = 3$

- $\Theta(:,:,k)$ slices $k = 1 : p$
- U^* is applied to all (np) columns
- V is applied to all (mp) rows
- U^*, V multiplications are well defined
- multiplications by matrix inverses are well defined

Slicing an $m \times n \times p$ Array Θ



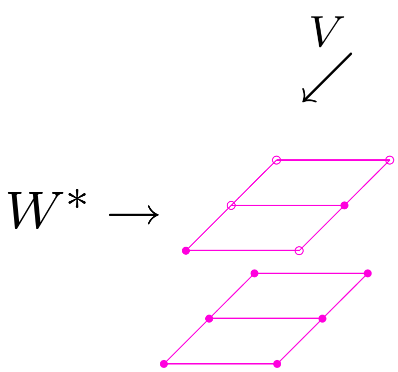
$$m = n = 2 \ , \ \ p = 3$$

- $\Theta(:, j, :)$ slices $j = 1 : n$

- U^* is applied to all (pn) columns

- W is applied to all (mn) rows

Slicing an $m \times n \times p$ Array $\ominus$



$$m = n = 2 \;\;,\;\; p = 3$$

- $(i, :, :)$ slices $i = 1 : m$

- W^* is applied to all (mn) columns

- V is applied to all (mp) rows

Tensor Product $\diamond$

A be a matrix
w be a vector

Define a tensor (3D array)

$$\Gamma = \mathbf{w} \diamond A$$

qualified by

$$\gamma_{ijk} \quad = \quad a_{ij} w_k$$

Alternatively,

$$\gamma_{ijk} \quad = \quad b_{ik} v_j \quad , \quad \Gamma = \mathbf{v} \diamond B$$

$$\gamma_{ijk} \quad = \quad c_{jk} u_i \quad , \quad \Gamma = \mathbf{u} \diamond C$$

Vectorizing Operator ν

Kronecker product: $\otimes$

$$
\begin{aligned}
\Gamma &= \mathbf{w} \diamond A \\
\nu_3\{\Gamma\} &= \mathbf{w} \otimes \nu_2\{A\} \\
\Gamma &= \nu_3^{-1}\{\mathbf{w} \otimes \nu_2\{A\}\}
\end{aligned}
$$

- **One tensor product $\rightarrow$ class 1**
- **$\nu\{.\}$ conserves all elements of $\{.\}$**
- **no information loss**
- **rearranged outer product**
- **inverse of ν is well defined**
- **an operator denoted by a single letter**

Flattening Operator $\flat$

$$
\begin{aligned}
\Gamma &= \mathbf{w} \diamond A \\
\flat\{\Gamma\} &= \mathbf{w} \otimes \nu\{A\}^t \\
\Gamma &= \flat^{-1}\{\mathbf{w} \otimes \nu\{A\}^t\}
\end{aligned}
$$

- $\flat$ conserves all elements of Γ
- no information loss
- inverse of $\flat$ is well defined

Tensor versus Kronecker

- $\otimes$ creates vectors out of vectors
- $\otimes$ creates matrices out of vectors
- $\otimes$ creates matrices out of matrices
- $\diamond$ creates new dimensions

An Example

$$A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \quad , \quad \mathbf{w} = \begin{bmatrix} w_1 \\ w_2 \\ w_3 \end{bmatrix}$$

$$\begin{aligned} \Gamma &= \mathbf{w} \diamond A \\ \gamma_{ijk} &= a_{ij} w_k \end{aligned}$$

Cross-sections wrt to the third dimension

$$\begin{aligned} \Gamma(:,:,1) &= w_1 A \\ \Gamma(:,:,2) &= w_2 A \\ \Gamma(:,:,3) &= w_3 A \end{aligned}$$

These are the natural cross-sections

Example Continued

$$\flat(\Gamma) = \begin{bmatrix} w_1 \\ w_2 \\ w_3 \end{bmatrix} \begin{bmatrix} a_{11} & a_{21} & a_{12} & a_{22} \end{bmatrix}$$

- $\nu(\Gamma)$ is a tall vector
- $\flat(\Gamma)$ is a rank-1 matrix

Cross-sections wrt Second Dimension

$$\begin{aligned}\Gamma(:,1,:) &= \begin{bmatrix} w_1 a_{11} & w_2 a_{11} & w_3 a_{11} \\ w_1 a_{21} & w_2 a_{21} & w_3 a_{21} \end{bmatrix}, \\ &= \begin{bmatrix} a_{11} \\ a_{21} \end{bmatrix} \mathbf{w}^t\end{aligned}$$

$$\begin{aligned}\Gamma(:,2,:) &= \begin{bmatrix} w_1 a_{12} & w_2 a_{12} & w_3 a_{12} \\ w_1 a_{22} & w_2 a_{22} & w_3 a_{22} \end{bmatrix} \\ &= \begin{bmatrix} a_{12} \\ a_{22} \end{bmatrix} \mathbf{w}^t\end{aligned}$$

- γ_{111} on the top left of $\Gamma(:,1,:)$
- reduced ranks in these cross-sections

Cross-sections wrt First Dimension

$$\Gamma(1,:,:) = \begin{bmatrix} w_1 a_{11} & w_2 a_{11} & w_3 a_{11} \\ w_1 a_{12} & w_2 a_{12} & w_3 a_{12} \end{bmatrix} = \begin{bmatrix} a_{11} \\ a_{12} \end{bmatrix} \mathbf{w}^t$$

$$\Gamma(2,:,:) = \begin{bmatrix} w_1 a_{21} & w_2 a_{21} & w_3 a_{21} \\ w_1 a_{22} & w_2 a_{22} & w_3 a_{22} \end{bmatrix} = \begin{bmatrix} a_{21} \\ a_{22} \end{bmatrix} \mathbf{w}^t$$

- γ_{111} on the top left of $\Gamma(1,:,:)$
- reduced ranks in these cross-sections

Cross-sections

- **implementation dependent**
- **we follow MATLAB and Fortran**
- **trivially different from De Lathauwer et al (2000)**
- $(1, 1, 1)$ **element at the top left**

Flattening with a Template

Arbitrary $\Theta \in \mathcal{C}^{m\times n\times p}$
Template $\Gamma \in \mathcal{C}^{m\times n\times p}$

$$\begin{aligned} \Gamma &= \mathbf{w} \diamond A \\ \flat\{\Gamma\} &= \mathbf{w} \otimes A^t \end{aligned}$$

Using the same element mapping rules

$$\begin{aligned} \flat\{\Theta\} &= F \\ \flat^{-1}\{F\} &= \Theta \end{aligned}$$

An Example

$$\flat\{\Gamma\} = \mathbf{w}\left[\begin{array}{cccc} a_{11} & a_{21} & a_{12} & a_{22} \end{array}\right]$$

$$\flat\{\Theta\} = \left[\begin{array}{cccc} \theta_{111} & \theta_{211} & \theta_{121} & \theta_{221} \\ \theta_{112} & \theta_{212} & \theta_{122} & \theta_{222} \\ \theta_{113} & \theta_{213} & \theta_{123} & \theta_{223} \end{array}\right]$$

Another 3D Class

a, b and c be vectors

We can define

$$\Gamma = \mathbf{a} \diamond \mathbf{b} \diamond \mathbf{c}$$

where

$$\gamma_{ijk} = a_i b_j c_k.$$

Two tensor products $\rightarrow$ class 2

Γ is rank 1

The Two 3D Classes

- Class 1 $\rightarrow$ Tucker/multilinear type model

- Class 2 $\rightarrow$ parafac/candecomp type model

Tucker (1966)
multilinear: De Lathauwer et al (2000)

parafac: Harshman (1970)
candecomp: Carroll and Chang (1970)

Orthogonal Vectors

$$
\begin{aligned}
U &= [\mathbf{u}^{(1)} \ldots \mathbf{u}^{(m)}] \quad , \quad U^*U = I \\
V &= [\mathbf{v}^{(1)} \ldots \mathbf{v}^{(n)}] \quad , \quad V^*V = I \\
W &= [\mathbf{w}^{(1)} \ldots \mathbf{w}^{(p)}] \quad , \quad W^*W = I
\end{aligned}
$$

In general, U, V and W are unitary

Three Linear Models for the Same Array

$$\Gamma \in \mathcal{C}^{m \times n \times p}$$

$$\Gamma \;=\; \sum_{k=1}^{p} \mathbf{w}^{(k)} \diamond A^{(k)}$$

$$\Gamma \;=\; \sum_{j=1}^{n} \mathbf{v}^{(j)} \diamond B^{(j)}$$

$$\Gamma \;=\; \sum_{i=1}^{m} \mathbf{u}^{(i)} \diamond C^{(i)}$$

- tensor summations

- Reminds one-sided Jacobi algorithms

Tensor from Core

The core array $\Sigma \in \mathcal{C}^{m \times n \times p}$

$$\Gamma_1 = \sum_{k=1}^{p} \mathbf{w}^{(k)} \diamond \Sigma(:,:,k)$$

$$\Gamma_2 = \sum_{j=1}^{n} \mathbf{v}^{(j)} \diamond \Gamma_1(:,j,:)$$

$$\Gamma = \sum_{i=1}^{m} \mathbf{u}^{(i)} \diamond \Gamma_2(i,:,:)$$

- tensor multiplications in any order
- can be extended to 4D and higher

Core from Tensor

Let $\widehat{\mathbf{w}}$ be the columns of $W^{-1} = W^*$

$$\Gamma_1 = \sum_{k=1}^{p} \widehat{\mathbf{w}}^{(k)} \diamond \Gamma(:,:,k)$$

$$\Gamma_2 = \sum_{j=1}^{n} \widehat{\mathbf{v}}^{(j)} \diamond \Gamma_1(:,j,:)$$

$$\Sigma = \sum_{i=1}^{m} \widehat{\mathbf{u}}^{(i)} \diamond \Gamma_2(i,:,:)$$

- tensor multiplications in any order

Core Orthogonality

$$\text{sum}\{\bar{\Sigma}(i_1, :, :) \circ \Sigma(i_2, :, :)\} = \alpha_1 \delta_{i_1 i_2}$$

$$\text{sum}\{\bar{\Sigma}(:, j_1, :) \circ \Sigma(:, j_2, :)\} = \alpha_2 \delta_{j_1 j_2}$$

$$\text{sum}\{\bar{\Sigma}(:, :, k_1) \circ \Sigma(:, :, k_2)\} = \alpha_3 \delta_{k_1 k_2}$$

Hadamard (Schur) product $\circ$
Element by element product $\circ$
Kronecker delta δ_{ij}

Core Orthogonality without $\circ$

$$\nu\{\Sigma(i_1,:,:)\}^*\nu\{\Sigma(i_2,:,:)\} \;=\; \alpha_1\delta_{i_1i_2}$$

$$\nu\{\Sigma(:,j_1,:)\}^*\nu\{\Sigma(:,j_2,:)\} \;=\; \alpha_2\delta_{j_1j_2}$$

$$\nu\{\Sigma(:,:,k_1)\}^*\nu\{\Sigma(:,:,k_2)\} \;=\; \alpha_3\delta_{k_1k_2}$$

Core Orthogonality

- Core in matrix SVD is diagonal

- Tucker model core is NOT diagonal

- Columns (rows) of matrix core are orthogonal

- Tucker model core slices are orthogonal

Tucker Model: Questions

Matrix SVD is optimal
Is Tucker model optimal ?

Explain core orthogonality

Best Rank One Approximation

Eckart-Young-Mirsky Problem

$$\min_{x,y} \|F - xy^*\|$$

$$\begin{aligned} \mathbf{x} &= \alpha\phi \\ \mathbf{y} &= (\sigma/\alpha)\psi \end{aligned}$$

- ϕ first left singular vector of F
- ψ first right singular vector of F
- σ first singular value of F
- $\alpha (= 1)$ arbitrary positive value
- similarly, the second best approximation

Best Rank k Approximation

Eckart-Young-Mirsky Problem

$$\min_{X,Y} \|F - XY^*\|$$

$$\begin{aligned} \mathbf{x}^{(i)} &= \phi^{(i)} \\ \mathbf{y}^{(i)} &= \sigma_i \psi^{(i)} \\ X &= [\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(k)}] \\ Y &= [\mathbf{y}^{(1)}, \ldots, \mathbf{y}^{(k)}] \end{aligned}$$

Tucker Model Algorithm

Arbitrary $\Theta \in \mathcal{C}^{m \times n \times p}$
Template $\Gamma = \mathbf{w} \diamond A$

$F = \flat\{\Theta\}$
Find $\mathbf{w}, A$ by $\quad \min \|F - \mathbf{w}\nu(A)^t\|$
number of solutions $= p$

$\Theta = \sum_{k=1}^{p} \mathbf{w}^{(k)} \diamond A^{(k)}$

Core Orthogonality

Due to the orthogonality of

$$A^{(k)}; \quad , \quad k = 1 : p$$

Tucker Singular values

- singular values of F for each template
- three possible templates in 3D

Complete Orthogonal Parafac

This is a decomposition

Not a model

Could be the SVD in 3D

Largest Singular Value of a Matrix

$$\sigma = \|A\|_2 \quad \text{primary definition}$$

$$= \max_{\|\mathbf{x}\|_2 = \|\mathbf{y}\|_2 = 1} \mathbf{x}^t A \mathbf{y}$$

$$\sigma^2 = \max_{\|\mathbf{y}\|_2 = 1} \mathbf{y}^t A^* A \mathbf{y}$$

$$= \max_{\|\mathbf{x}\|_2 = 1} \mathbf{x}^t A A^* \mathbf{x}$$

$\mathbf{x} \in \mathcal{C}^m \;,\; \mathbf{y} \in \mathcal{C}^n$

Largest Singular Value of a 3D Array ?

$\mathbf{x} \in \mathcal{C}^m \ , \ \mathbf{y} \in \mathcal{C}^n \ , \ \mathbf{z} \in \mathcal{C}^p$

$$\begin{aligned}
\sigma_{3D} &= \max_{\|\mathbf{x}\|_2 = \|\mathbf{y}\|_2 = \|\mathbf{z}\|_2 = 1} \sum_{k=1}^{p} z_k \mathbf{x}^t \Theta(:,:,k) \mathbf{y} \\
&= \max_{\|\mathbf{x}\|_2 = \|\mathbf{y}\|_2 = \|\mathbf{z}\|_2 = 1} \sum_{i=1}^{m} \sum_{j=1}^{n} \sum_{k=1}^{p} \theta_{ijk} x_i y_j z_k
\end{aligned}$$

This is a reasonable secondary definition

see Zhang and Golub (2001)

What is the primary definition ?

Sets of Matrices

$$\begin{aligned}
\mathcal{A} &= \{A_1, A_2, \ldots A_p\} \\
\mathcal{B} &= \{B_1, B_2, \ldots B_p\} \\
\alpha\mathcal{A} &= \{\alpha A_1, \alpha A_2, \ldots \alpha A_p\} \\
\mathcal{A} + \mathcal{B} &= \{A_1 + B_1, A_2 + B_2, \ldots A_p + B_p\}
\end{aligned}$$

A Norm for a Set of Matrices

Define the function μ,

$$\mu(\mathcal{A}) \;=\; \max_{\|\mathbf{z}\|_2=1} \|\sum_{k=1}^{p} z_k A_k\|_2$$

Then

$$\mu(\mathcal{A}) \;\geq\; 0$$

$$\mu(\mathcal{A}) \;=\; 0 \;\rightarrow \mathcal{A} = 0$$

$$\mu(\alpha\mathcal{A}) \;=\; |\alpha|\mu(\mathcal{A})$$

$$\mu(\mathcal{A}+\mathcal{B}) \;\leq\; \mu(\mathcal{A}) + \mu(\mathcal{B})$$

Thus, $\mu(.)$ is a norm induced by the 2-norm

A Norm for a 3D Array

Can be defined via the slices

$$\begin{aligned}
\mu(\Theta) &= \max_{\|\mathbf{z}\|_2=1} \| \sum_{k=1}^{p} z_k \Theta(:,:,k) \|_2 \\
&= \max_{\|\mathbf{y}\|_2=1} \| \sum_{j=1}^{m} y_k \Theta(:,j,:) \|_2 \\
&= \max_{\|\mathbf{x}\|_2=1} \| \sum_{i=1}^{n} x_k \Theta(i,:,:) \|_2 \\
&= \max_{\|\mathbf{x}\|_2=\|\mathbf{y}\|_2=\|\mathbf{z}\|_2=1} \sum_{i=1}^{m} \sum_{j=1}^{n} \sum_{k=1}^{p} \theta_{ijk} x_i y_j z_k
\end{aligned}$$

A Bound for the Norm

$$\mu(\Theta) \leq \sqrt{\sum_{k=1}^{p} \|\Theta(:,:,k)\|_2^2}$$

$$\mu(\Theta) \leq \sqrt{\sum_{j=1}^{n} \|\Theta(:,j,:)\|_2^2}$$

$$\mu(\Theta) \leq \sqrt{\sum_{i=1}^{m} \|\Theta(i,:,:)\|_2^2}$$

Invariant Property

$$
\begin{aligned}
\mu\left(\sum_{k=1}^{p} \mathbf{w}^{(k)} \diamond \Theta(:,:,k)\right) &= \mu(\Theta) \\
\mu\left(\sum_{j=1}^{n} \mathbf{v}^{(j)} \diamond \Theta(:,j,:)\right) &= \mu(\Theta) \\
\mu\left(\sum_{i=1}^{m} \mathbf{u}^{(i)} \diamond \Theta(i,:,:)\right) &= \mu(\Theta)
\end{aligned}
$$

where U, V and W are unitary

Three Subproblems

$$\mu(\Theta) \;=\; \max_{\|\mathbf{z}\|_2=1} \| \sum_{k=1}^{p} z_k \Theta(:,:,k) \|_2$$

- μ_{cc} $\leftarrow$ **Θ and $\mathbf{z}$ are complex (generic)**

- μ_{rc} $\leftarrow$ **Θ is real and $\mathbf{z}$ is complex**

- μ_{rr} $\leftarrow$ **Θ and $\mathbf{z}$ are real**

A Surprising Result

$$\mu_{rr}(\Theta) \;\leq\; \mu_{rc}(\Theta)$$

The following statements are wrong

- Without loss of generality we assume that the array is real

- This can be easily extended to the complex case

An Algorithm for the Largest Singular Value

$\Theta \in \mathcal{C}^{m \times m \times m}$

Use permutations to make $|\theta_{111}|$ the largest (permutation matrices are unitary)

$[U, S, V] = svd(\Theta(:, :, 1))$
Apply U^* and V to Θ

$[U, S, W] = svd(\Theta(:, 1, :))$
Apply U^* and W to Θ

$[W, S, V] = svd(\Theta(1, :, :))$
Apply W^* and V to Θ

Repeat above until convergence

Convergence

Element θ_{111} does not increase

The three edges

$\Theta(1, 1, :)$
$\Theta(1, :, 1)$
$\Theta(:, 1, 1)$

are zero except for the element θ_{111}

An Algorithm for the Second Singular Value

Use permutations to make $|\theta_{222}|$ the largest without disturbing θ_{111}

$[U, S, V] = svd(\Theta(2:m, 2:m, 2))$
Apply U^* and V to Θ

$[U, S, W] = svd(\Theta(2:m, 2, 2:m))$
Apply U^* and W to Θ

$[W, S, V] = svd(\Theta(2, 2:m, 2:m))$
Apply W^* and V to Θ

Repeat above until convergence

Convergence

Element θ_{222} does not increase

The three edges

$\Theta(2, 2, 3 : m)$
$\Theta(2, 3 : m, 2)$
$\Theta(3 : m, 2, 2)$

are zero

The 3D SVD

For $\Theta \in \mathcal{C}^{m\times m\times m}$

$$\Theta = \sum_{i}^{m}\sum_{j}^{m}\sum_{k}^{m} \pi_{i,j,k}\mathbf{u}^{(i)} \diamond \mathbf{v}^{(j)} \diamond \mathbf{w}^{(k)}$$

where

$\pi_{q,q,q}$
for $q = 1 : m$ are the 'singular values'

The edges:

$\pi_{q+1:m,q,q} = 0$
$\pi_{q,q+1:m,q} = 0$
$\pi_{q,q,q+1:m} = 0$

for $q = 1 : m-1$

Main Properties

$$\begin{aligned}
\pi_{1,1,1} &\geq \pi(1, j, k) \\
&\geq \pi(i, 1, k) \\
&\geq \pi(i, j, 1)
\end{aligned}$$

Main Properties

$$\begin{aligned}\pi_{1,1,1} &\geq \sigma\{\Pi(1, 2:m, 2:m)\} \\ &\geq \sigma\{\Pi(2:m, 1, 2:m)\} \\ &\geq \sigma\{\Pi(2:m, 2:m, 1)\}\end{aligned}$$

$\pi_{2,2,2}$

Peel off the first layer

Use properties of $\pi_{1,1,1}$

Monotonicity

$$\pi_{1,1,1} \geq \pi_{2,2,2} \geq \pi_{3,3,3} \geq \ldots$$

Orthogonal Rank ?

Number of non-zero $\pi_{q,q,q}$

Conclusions: Tucker Model

- 3D Tucker is based on 3 SVDs
- Tucker model is optimal
- Three ways to express the same model
- Eckart-Young-Mirsky (EYM) in 3 ways
- Core orthogonality due to EYM
- only one tensor (outer) product
- one-sided Jacobi expansions

Conclusions: 3D Norm

- A norm induced by the vector 2-norm
- Compatible with Zhang-Golub
- Computable bounds for the norm
- Generic problem is complex

Conclusions: 3D SVD

- Based recursively on the 3D norm
- Complete orthogonal parafac
- Two tensor products
- Edges are zero
- Diagonals give 'ordered singular values'
- Off-diagonals give 'sub-singular values'

Conclusions: Tensor Classes

- Tucker is class 1

- 3D parafac is class 2

- Vector spaces are vectors, matrices 3D arrays etc

- Tensors are products of vector spaces

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